AD-A185 405

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION	1b. RESTRICTIVE MARKINGS
Unclassified	

2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT
	Approved for public release;
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	distribution unlimited

4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
Mathematical Research Report #86-2	AFOSR·TR· 87 - 1036

6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
University of Maryland Baltimore County	UMBC	Air Force Office of Scientific Research

6c. ADDRESS (City, State and ZIP Code)	7b. ADDRESS (City, State and ZIP Code)
Department of Mathematics Catonsville, Maryland 21228	Directorate of Mathematics and Information Sciences Bolling AFB, D.C. 20332-6448

8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
AFOSR	NM	AFOSR -85-0322

8c. ADDRESS (City, State and ZIP Code)	10. SOURCE OF FUNDING NOS.			
Directorate of Mathematics and Information Sciences Bolling AFB D. C. 20332 - 6448	PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.
	61102 F	2304	A	

11. TITLE (Include Security Classification) Numerical Methods for Reaction-Diffusion-Problems with Non-Differentiable Kinetics [Unclassified]

12. PERSONAL AUTHOR(S)
A. K. Aziz, A. B. Stephens, M. Suri

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Yr., Mo., Day)	15. PAGE COUNT
Summary	FROM No Specific Time	86, 11, 7	21

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	Reaction-Diffusion problems, semilinear equations, finite elements, finite differences, error estimates.
12.01			

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This document The We consider a class of steady-state semilinear reaction-diffusion problems with non-differentiable kinetics. The analytical properties of these problems have received considerable attention in the literature. We take a first step in analyzing their numerical approximation. We present a finite element method and establish error bounds which are optimal for some of the problems. In addition, we also discuss a finite difference approach. Numerical experiments for one-and two-dimensional problems are reported. are also discussed. A In Taxon, The author

87 9 24 319

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS ☐	Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE NUMBER (Include Area Code)	22c. OFFICE SYMBOL
John P. Thomas, Jr., Capt., USAF	(202) 767-5025	AFOSR/NM

DD FORM 1473, 83 APR   EDITION OF 1 JAN 73 IS OBSOLETE.   Unclassified

Mathematics Research Reports

AFOSR·TR· 87 - 1 0 3 6

NUMERICAL METHODS FOR REACTION-DIFFUSION PROBLEMS

WITH NON-DIFFERENTIABLE KINETICS

A. K. Aziz[1,2]

A. E. Stephens[2]

Manil Suri[2,3]

Dedicated to Ivo Babuska on his sixtieth birthday

Mathematics Research Report #86-2

Department of Mathematics

UNIVERSITY OF MARYLAND
BALTIMORE COUNTY

Catonsville, Maryland 21228

DTIC

ELECTE

OCT 0 6 1987

S

E

NUMERICAL METHODS FOR REACTION-DIFFUSION PROBLEMS

WITH NON-DIFFERENTIABLE KINETICS

A. K. Aziz[1,2]

A. B. Stephens[2]

Manil Suri[2,3]

Dedicated to Ivo Babuška on his sixtieth birthday

Accession For	
NTIS GRA&I	☑
DTIC TAB	☐
Unannounced	☐
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

DTIC COPY INSPECTED 6

[1] Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742.

[2] University of Maryland, Baltimore County, Catonsville, MD 21228.

Abstract

We consider a class of steady-state semilinear reaction-diffusion problems with non-differentiable kinetics. The analytical properties of these problems have received considerable attention in the literature. We take a first step in analyzing their numerical approximation. We present a finite element method and establish error bounds which are optimal for some of the problems. In addition, we also discuss a finite difference approach. Numerical experiments for one- and two-dimensional problems are reported.

1. Introduction

The problem we consider is that of an irreversible steady-state reaction taking place in a bounded domain Ω in R^n (n = 1,2,3) with smooth boundary $\partial\Omega$. The reason a steady-state occurs is that the reactant used up in the reaction in Ω is replenished by diffusion from the surrounding region. In [1], it is shown that the problem may be modeled by a scalar equation for the concentration alone:

$$(1.1) \qquad \Delta u = \lambda f(u(x)), \qquad x \in \Omega \qquad\qquad (u \geq 0 \text{ in } \Omega)$$

$$u = 1 \qquad\qquad x \in \partial\Omega$$

where λ is a positive constant that measures the ratio of reaction to diffusion rates. The function f measures the ratio of the reaction rate at concentration u to that at concentration unity. We assume that the function f satisfies the following conditions:

$$(1.2) \qquad f(t) = 0 \text{ if } t \leq 0, \quad f(1) = 1$$

$$(1.3) \qquad f(t) = t^p f_0(t) \text{ for } 0 \leq t < \infty, \qquad 0 < m \leq f_0(t) \leq M < \infty$$

$$|f_0{}''(t)| \leq K, \quad 0 < p < 1$$

$$(1.4) \qquad f'(t) + \frac{f(t)}{1-t} > 0 \quad \text{for } 0 < t \leq 1.$$

For the case of a non-isothermal reaction, we may obtain the temperature v of the reactant from the relation

$$(1.5) \qquad v = \beta(1-u) + 1$$

where $\beta > 0$ if the reaction is exothermic and $\beta < 0$ if it is endothermic. We will primarily be interested in the isothermal case $(\beta = 0)$,

when v remains identically unity [u and v are nondimensional variables].

The problem (1.1) has been discussed in an analytical framework in [1] and [3]. An interesting feature analyzed in these papers is the existence of a "dead core," i.e., a region in Ω where u identically vanishes, for p <1 and λ large enough. Physically, this means that the rate of reaction is so high that the reactant is being consumed in the dead core faster than it can be replaced through diffusion across the boundary $\partial\Omega$.

The goal of this paper is to take a first step in approximating (1.1) numerically. We will analyze numerical schemes only for the case of <u>pth order isothermal reactions</u>, for the case 0 < p < 1, where f is explicitly given by:

(1.6) $\qquad\qquad f(t) = t^p \qquad$ for t > 0

$\qquad\qquad\qquad\quad = 0 \qquad$ for t $\leq$ 0.

It can be seen that this function satisfies (1.2) - (1.4)

For p $\geq$ 1, this nonlinear problem may be approximated by several methods (for e.g. [2], [4]). However, when p < 1, f is not differentiable at the origin (and if p = 0, it is not even continuous there). Hence, the convergence theorems in the above papers fail and a different analysis is required for the case of non-differentiable kinetics.

The plan of the paper is as follows. In Section 2, we list existence, uniqueness and regularity results from [1] and [3] that will be needed. In Section 3, we present a finite element method for (1.1) and obtain an error estimate for its convergence. In Section 4, we discuss a finite

difference scheme for the problem. Section 5 contains the results of numerical experiments using our schemes.

2. Existence, Uniqueness and Regularity Theorems

The following theorem is proved in [3].

Theorem 2.1. Let f satisfy (1.2) - (1.4). Let Ω have a C^{2,α_0} boundary $\partial\Omega$. Then there exists a unique solution of (1.1) belonging to $C^{2,\alpha}(\bar{\Omega})$ where $\alpha = \min(p, \alpha_0)$.

Since the function f given by (1.6) satisfies (1.2) - (1.4), the above theorem holds for this function. In [1], an alternate proof of existence and uniqueness is provided, where conditions (1.3) - (1.4) are replaced by the requirement that f is positive, continuously differentiable and monotone increasing on $(0,\infty)$. This provides results for the function f in (1.6) for all $p \geq 0$.

By the maximum principle, it follows readily that $u \leq 1$ in Ω. Moreover, the condition (1.2) ensures that $u \geq 0$ in Ω, which is essential in terms of physical considerations.

For a convex two-dimensional domain, the dead-core, if it exists, will be convex. The existence of the dead core depends on the parameter λ, as expressed in the following theorem, a slightly modified version of which is proved in [1].

Theorem 2.2. Let f satisfy (1.3). Then there exists a number $\lambda_0 > 0$ such that (1.1) has a dead core for all $\lambda \geq \lambda_0$.

If λ is small enough or if $p \geq 1$, then no dead core will exist. For the case of a pth order isothermal reaction in a slab, where $\bar{\Omega} =$

[-d,d] (d is the width of the slab) and f is given by (1.6), the dead core appears only if

$$(2.1) \qquad \sqrt{\lambda} > \frac{A}{d} \quad \text{where} \quad A = \frac{\sqrt{2}\,\sqrt{p+1}}{1-p} \qquad (0 \le p < 1).$$

Moreover, the size of the dead core $D_0 = [-\gamma, \gamma]$ is determined by

$$(2.2) \qquad \gamma = d - \frac{A}{\sqrt{\lambda}}.$$

Similarly, for a pth order isothermal reaction in a ball, there is a critical value λ_0 such that a dead core appears if and only if $\lambda \ge \lambda_0$. The above facts are proved in [1], where several other theorems for the existence and non-existence of a dead core are provided.

Finally, it is shown in [3] that asymptotically, as $\lambda \to \infty$, the boundary of the dead core approaches a smooth surface parallel to $\partial\Omega$ at distance $\frac{\delta}{\sqrt{\lambda}} + O(\frac{1}{\lambda})$, δ constant.

3. A Finite Element Approximation

For convenience, we make the substitution $v = 1 - u$ in (1.1), (1.6). This yields the problem

$$(3.1) \qquad -\Delta v = \lambda g(v) \quad \text{in} \quad \Omega$$

$$v = 0 \quad \text{on} \quad \partial\Omega$$

where

$$(3.2) \qquad g(v) = (1-v)^p \quad \text{for} \quad v \le 1, \qquad p \in (0,1)$$

$$= 0 \qquad \text{for} \quad v > 1$$

We know that (3.1) has a unique solution $v \in H^2(\Omega)$, $0 \leq v \leq 1$ where the region $G = \{x \mid v(x) = 1\}$ corresponds to the dead core. The equivalent weak formulation of (3.1) is given by:

Find $v \in H_0^1(\Omega)$ satisfying

$$(3.3) \qquad (\nabla v, \nabla w) = \lambda(g(v), w) \quad \text{for all} \quad w \in H_0^1(\Omega)$$

where $(\cdot, \cdot)$ denotes the usual $L^2(\Omega)$ inner product.

Let now S^h be a finite dimensional subspace of $H_0^1(\Omega)$ with the property

$$(3.4) \qquad \inf_{\chi \in S^h} \{|v - \chi|_0 + h|v - \chi|_1\} \leq Ch^s |v|_s \quad \text{for} \quad 1 \leq s \leq r + 1.$$

Here r denotes the degree of piecewise polynomials used. Since our solution is only known to lie in $H^2(\Omega)$, we restrict attention to the case $r = 1$ so that S^h consists simply of piecewise linear functions.

We say that $v^h \in S^h$ is an approximate solution of (3.1) if

$$(3.5) \qquad (\nabla v^h, \nabla w^h) = \lambda(g(v^h), w^h) \qquad \forall w^h \in S^h.$$

Theorem 3.1. Let g be given by (3.2). Then there exists a function $v^h \in S^h$ satisfying (3.5).

The proof of Theorem 3.1 requires the following lemmas:

Lemma 3.1. Let M_n be a finite dimensional space and let $T : M_n \to M_n$ be continuous. Suppose there exists a sphere S_ρ with radius ρ and center at the origin such that $(Tx, x) \geq 0$ for x on S_ρ. Then there exists an x_0 such that $Tx_0 = 0$ and $|x_0| \leq \rho$.

Proof: See, for example, [7].

Lemma 3.2. Let g be given by (3.2). Then for any $v_1, v_2 \in R$,

$$(3.6) \qquad |g(v_1) - g(v_2)| \leq |v_1 - v_2|^p.$$

Proof. We may assume without loss of generality that $v_1 > v_2$. [If $v_1 = v_2$, (3.6) holds trivially.] If $v_1 \geq 1$, then we see that

$$|g(v_1) - g(v_2)| \leq |g(v_2)| \leq |1 - v_2|^p \leq |v_1 - v_2|^p.$$

If $v_1 < 1$, then

$$0 \leq 1 - v_1 < 1 - v_2$$

so that

$$0 \leq \frac{1 - v_1}{1 - v_2} = a < 1.$$

Hence, $1 - a^p \leq 1 - a \leq (1-a)^p$, since $0 < p < 1$. This gives

$$(1-v_2)^p - (1-v_1)^p \leq (v_1 - v_2)^p$$

and (3.6) is proven.

Lemma 3.3. Let $0 < p < 1$. Then for $v \geq 0$, $\quad v, w \in L^2(\Omega)$,

$$(3.7) \qquad |(v^p, w)| \leq c|v|_0^p |w|_0.$$

Proof. Using the Schwarz inequality, we have

$$|(v^p, w)| \leq c \left(\int_\Omega (v^p)^2 dx \right)^{\frac{1}{2}} |w|_0.$$

Now by Hölder's inequality with $q = \dfrac{1}{p}$ and $\dfrac{1}{r} + \dfrac{1}{q} = 1$,

$$\int_\Omega v^{2p}dx \leq \left(\int_\Omega (v^{2p})^q dx\right)^{1/q} \left(\int_\Omega 1^r dx\right)^{1/r}$$

$$\leq C\left(\int_\Omega v^2 dx\right)^{1/q}$$

from which (3.7) follows.

Proof of Theorem 3.1.

Define an operator $T : S^h \to S^h$ as follows:

$$(Tv^h, w^h) = (\nabla v^h, \nabla w^h) - \lambda(g(v^h), w^h) \quad \text{for all} \quad w^h \in S^h.$$

Clearly T is continuous. Moreover, using (3.7),

$$(Tv^h, v^h) \geq |\nabla v^h|_0^2 - C\lambda|1 - v^h|_0^p |v^h|_1$$

$$\geq C(|v_1^h|^2 - \lambda[A^p + |v_1^h|^p]|v_1^h|)$$

where $A =$ measure of Ω. Hence, for $|v^h|_1 = \rho$ sufficiently large, we have

$$(Tv^h, v^h) \geq 0.$$

Applying Lemma 3.1 yields the theorem.

Theorem 3.2. (3.5) has a unique solution. Moreover, for S^h consisting of piecewise linear functions, the solution $v^h \geq 0$ on Ω.

Proof. We first prove uniqueness. let v_1^h and v_2^h be two solutions of (3.5) and let $w^h = v_2^h - v_1^h$. Then, from (3.5) we have:

$$(\nabla w^h, \nabla w^h) = \lambda(g(v_2^h) - g(v_1^h), v_2^h - v_1^h).$$

Since $g(v)$ is decreasing in v, it follows that

$$|\nabla w^h|_0^2 \leq 0.$$

Since $w^h = 0$ on $\partial\Omega$, this implies $w^h = 0$, that is $v_1^h = v_2^h$. Let now v^h, the solution of (3.5) satisfy

$$v^h(N_i) < 0$$

for some nodal point N_i in the grid on Ω. Then there exists a nodal point N_0 such that

(3.8a) $\quad v^h(N_0) \leq v^h(x) \quad$ for all $x \in \Omega$.

(3.8b) $\quad v^h(N_0) < 0$

(3.8c) $\quad v^h(N_0) < v^h(N_j) \quad$ for at least one node N_j adjacent to N_0

$\qquad\qquad\qquad\qquad\qquad$ (since $v^h = 0$ on $\partial\Omega$).

Now, let ψ_0 be the linear basis function that is 1 at the point N_0 and 0 at all other nodal points, and let Ω_0 be its support. Then, by (3.8a), ∇v^h is of the opposite sign as $\nabla\psi_0$ on Ω_0 and by (3.8c), ∇v^h is not identically zero on Ω_0. Hence, substituting $w^h = \psi_0$ in (3.5), we obtain

$$(\nabla v^h, \nabla\psi_0) = \int_{\Omega_0} \nabla v^h \cdot \nabla\psi_0 dx = \lambda(g(v^h), \psi_0).$$

The left side is strictly negative while the right side is non-negative, a contradiction.

Remark. The non-negativity proof above is essentially the discrete maximum principle (using linear functions) for the non-linear problem (3.1) with non-negative forcing function g.

We now deal with the question of convergence of v^h to v.

Theorem 3.3. Let v^h be the solution of (3.5) and v the solution of (3.3). Then

$$\left| v - v^h \right|_1 \leq Ch \qquad \text{if } \frac{1}{2} \leq p < 1$$

$$\leq Ch^{2p} \qquad \text{if } 0 < p < \frac{1}{2}$$

where the constant C is independent of h but depends on u, λ, p and Ω.

Proof. Let χ be as in (3.4) and $w^h \in S^h$. Then, by (3.3), (3.5), we have

$$(3.9) \qquad (\nabla(v^h-\chi), \nabla w^h) + (g(\chi)-g(v^h), w^h)$$

$$= (\nabla(v-\chi), \nabla w^h) + (g(\chi)-g(v), w^h).$$

Taking $w^h = v^h - \chi$ in (3.9) gives

$$(3.10) \qquad \left| \nabla(v^h-\chi) \right|_0^2 + (g(\chi)-g(v^h), v^h-\chi)$$

$$= (\nabla(v-\chi), \nabla(v^h-\chi)) + (g(\chi)-g(v), v^h-\chi).$$

Since $g(v)$ is decreasing for $v \leq 1$ and zero for $v > 1$, it follows that

$$(g(\chi)-g(v^h), v^h-\chi) \geq 0.$$

Hence, we may obtain from (3.10):

$$\left\| \nabla(v^h - \chi) \right\|_0^2 \leq \left\| \nabla(v - \chi) \right\|_0 \left\| \nabla(v^h - \chi) \right\|_0 + (g(\chi) - g(v), v^h - \chi).$$

Using (3.6), (3.7) and the Poincaré inequality gives

$$\left| v^h - \chi \right|_1 \leq \left| v - \chi \right|_1 + c\sqrt{\lambda} \left| v - \chi \right|_0^p).$$

Using the approximation property (3.4) together with the triangle inequality yields

$$(3.11) \qquad \left| v - v^h \right|_1 \leq C(h \left| v \right|_2 + \sqrt{\lambda} \, h^{2p} \left| v \right|_2^p)$$

from which the assertion of the theorem follows.

Remark. The estimate given in Theorem 3.3 for the case $p < \frac{1}{2}$ is pessimistic. The numerical experiments in Section 5 suggest that one gets $O(h)$ convergence for any p.

4. A Finite Difference Approach

In this section, we present a finite difference scheme for (1.1), (1.6) and analyze its numerical properties.

For the sake of our discussion, we take Ω to be the unit square $0 \leq x \leq 1$, $0 \leq y \leq 1$.

Let Ω_h be a uniform $n \times n$ finite difference mesh with mesh spacing h and boundary $\partial \Omega_h$. $u_{i,j}$ will indicate an approximate value of the solution of (1.1), (1.6) at $(x_i, y_j) \equiv (ih, jh)$ for $0 \leq i,j \leq N$. $\bar{u}_h$ will denote the vector with components $u_{i,j}$, $1 \leq i,j \leq N - 1$, listed row by row.

Let Δ_h be the usual five-point discrete Laplacian and consider the scheme

$$(4.1) \qquad \Delta_h \alpha_h = \lambda \alpha_h^p \text{ on } \Omega_h, \qquad \alpha_h = 1 \text{ on } \partial\Omega_h.$$

Let $m = (N-1)^2$ and let $R^{m+} = \{\mathbf{x} \mid 0 \leq x_i, \ i = 1,\dots,m\}$. Then (4.1) may be expressed as a non-linear system of m equations in m unknowns:

$$(4.2) \qquad \tilde{F}(\alpha_h) = \{F_{ij}(\alpha_h)\} = \tilde{b}$$

where F_{ij} is defined on R^{m+} for $2 \leq i,j \leq N-2$ by

$$(4.3) \quad F_{ij}(\alpha_h) = -u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} + 4u_{i,j} + \lambda h^2 u_{i,j}^p.$$

For other values of i,j, F_{ij} is defined once again by (4.3) except that the contributions from $u_{i,j}$ on $\partial\Omega_h$ are taken on the right hand side to comprise the vector $\tilde{b}$. Notice that all entries in $\tilde{b}$ will be non-negative. In what follows, we will assume for simplicity that the components of $\tilde{F}$ and α_h are given by $\{F_i\}$ and $\{u_i\}$ respectively, $i = 1,2,\dots,m$. We will be using the terminology from [5] and [6] to define terms like inverse isotone, off-diagonally antitone and M-function.

The continuous mapping $\tilde{F} : R^{m+} \to R^m$ turns out to be an M-function, yielding the following result.

Theorem 4.1. The difference scheme (4.1) has a unique solution $0 \leq \alpha_h \leq 1$. Moreover, let $\alpha_1^0, \alpha_2^0 \in R^{m+}$ be vectors with all components 0 and 1, respectively. For any $\omega \in (0,1]$ define the (SOR) iterates α^k by

$$F_i(u_1^{k+1},\ldots,u_{i-1}^{k+1},u_i^k,u_{i+1}^k,\ldots,u_m^k) \;=\; b_i \quad \text{for} \;\; u_i,$$

(4.4)

$$u_i^{k+1} \;=\; u_i^k + \omega(u_i - u_i^k); \qquad\qquad i = 1,2,\ldots,m, \quad k = 0,1,\ldots$$

Then the iterates $\{u^k\}$ starting from u_1^0 and u_2^0 are uniquely defined, non-negative and converge monotonically to u_h from below and above, respectively.

   Proof. We first show that F is an M-function. By Def. 2.8 of [6], we must show that F is inverse isotone and off-diagonally antitone. Define $\tilde{\phi} : R^{m+} \to R^m$ by

(4.5) $$\phi_i(u_h) \;=\; \lambda h^2 u_i, \qquad\qquad 1 \le i \le m.$$

Then it is immediately seen that $\tilde{\phi} : R^{m+} \to R^m$ is a continuous, isotone, diagonal mapping. Moreover, (4.3), (4.5) may be used to obtain the following splitting for $\tilde{F}$:

(4.6) $$\tilde{F}(u_h) \;=\; Au_h + \tilde{\phi}(u_h).$$

   The $m \times m$ matrix A is irreducibly diagonally dominant with $a_{i,j} \le 0$ for $i \ne j$ and $a_{i,i} > 0$ for $i = 1,\ldots,n$. From this, it follows that $\tilde{F}$ if off-diagonally antitone. In addition, by 2.4.14, p. 55 of [5], A is an M-matrix. The fact that F is inverse isotone now follows easily by the proof of 13.5.6, p. 467 of [5].

   By Theorem 2.10 of [6], F is strictly diagonally isotone. We now note that taking x_0, $y_0 \in R^{m+}$ consisting of all 0's and all 1's, respectively, yields

$$x_0 \;\le\; y_0$$

$$\tilde{F}(\tilde{x}_0) \leq \tilde{b} \leq \tilde{F}(\tilde{y}_0)$$

and

$$J = \{x \in \mathbb{R}^n \mid x^0 \leq x \leq y^0\} \subset \mathbb{R}^{m+}.$$

By Theorem 3.1 of [6], we find that for any $\omega \in (0,1]$, the Gauss-Seidel iterates $\{\tilde{y}_k\}$ and $\{\tilde{x}_k\}$ given by (4.4) and starting from $\tilde{y}_0$ and $\tilde{x}_0$, respectively, are uniquely defined and satisfy $\tilde{x}_k \to \tilde{x}^*$, $\tilde{y}_k \to \tilde{y}^*$, $\tilde{F}(\tilde{x}^*) = \tilde{F}(\tilde{y}^*) = \tilde{b}$, where the monotonicity of the convergence insures $0 \leq x_i^*, y_i^* \leq 1$, $i = 1,2,\ldots,m$. Finally, the fact that $\tilde{x}^* = \tilde{y}^* = \tilde{U}_h$ follows from the inverse isotonicity of $\tilde{F}$, so that $\tilde{U}_h$ is unique and $0 \leq \tilde{U}_h \leq 1$.

Remark: It is obvious that Theorem 4.1 will be true for any sub and super solutions U_1^0 and U_2^0, respectively, for (4.2).

(4.4) therefore provides us with an iterative scheme to solve (4.1) which has been used successfully by us in computations. It is of interest to note that the solution $\tilde{U}_h$ of (4.1) does not have a discrete dead core in the sense that $u_{i,j} \neq 0$ at any point of the mesh. For, if $u_{i,j} = 0$ at a mesh point, then by (4.3) we obtain

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} = 0$$

so that by non-negativity of the solution,

$$u_{i-1,j} = u_{i+1,j} = u_{i,j-1} = u_{i,j+1} = 0.$$

This in turn implies that $\tilde{U}_h = 0$ at all interior mesh points, a consequence that obviously contradicts (4.1) adjacent to $\partial\Omega_h$.

Numerical experiments show that the above difference scheme yields

O(h) convergence in the discrete H^1 norm of the error. As for many difference schemes, a higher convergence rate is obtained if it is measured at the nodes alone. The following difference scheme for the one-dimensional problem is interesting in this respect.

$$(4.5) \qquad u_{i+1} - 2u_i + u_{i-1} = \lambda h^2 \left(\frac{u_{i+1}^p + 10u_i^p + u_{i-1}^p}{12} \right).$$

For the case when $\lambda = 12$ and $p = \frac{1}{2}$, (4.5) reproduces the true solution $u = x^4$ exactly at the mesh points, so that the error is zero at these points.

5. Numerical Experiments

In this section we look at results obtained using the finite element method. In the one-dimensional case, the width of the dead core for (1.1), (1.6) can be analytically determined by (2.1), (2.2). Moreover, when $\Omega = [-1,+1]$, $p = 0.5$ and $\lambda = 12$, the exact solution is given by $u = x^4$, which has a one-point dead core at the origin. In this case, the error in the computations below can be measured exactly. In other cases, the true solution is replaced by an approximation using a sufficiently small mesh size [number of sub-intervals, $N = 64$]. The mesh size h is given by $2/N$.

p	λ	N	H^1 error
0.5	12	4	1.0438
		8	0.5450
		12	0.3610
		16	0.2735
0.5	20	4	1.4404
		8	0.7923
		12	0.5387
		16	0.3957
0.1	20	4	1.9429
		8	1.0071
		12	0.6827
		16	0.5035

The above experiments show the errors obtained with linear elements. It is observed that the rate of convergence in the H^1 norm is $O(h)$ in all cases. This corresponds with the estimates for $p \geq 0.5$ in Theorem 3.3 but exceeds the rate of $O(h^{2p})$ predicted for $p < 0.5$.

The two-dimensional results show exactly the same orders of convergence. In this case, experiments are first performed over a square using linear piecewise polynomials on a uniform triangular mesh. The next set of experiments involve bilinear functions on a uniform rectangular mesh. Both these finite element spaces satisfy (3.4). N now represents the number of sub-divisions on each side of the square and the mesh size h is once again 2/N. Some sample results are presented below.

Linear Functions

p	λ	N	H^1 error
0.5	4	4	0.5485
		8	0.2845
		12	0.1910
		16	0.1407
	24	4	2.1017
		8	1.1250
		12	0.9330
		16	0.5676
	48	4	3.0907
		8	1.8063
		12	1.1848
		16	0.9130
0.1	4	4	0.6155
		8	0.3177
		12	0.2140
		16	0.1569
	10	4	1.5497
		8	0.8694
		12	0.6600
		16	0.5393
	20	4	2.3220
		8	1.2086
		12	0.8128
		16	0.6024

Bilinear Functions

p	λ	N	H^1 error
0.5	4	4	0.4022
		8	0.2030
		12	0.1352
		16	0.0995
	24	4	1.7751
		8	0.9312
		12	0.6149
		16	0.4596
	48	4	2.8526
		8	1.6228
		12	1.0570
		16	0.8051
0.1	4	4	0.4382
		8	0.2200
		12	0.1468
		16	0.1077
	10	4	1.1021
		8	0.5718
		12	0.4046
		16	0.3145
	20	4	1.9706
		8	0.9848
		12	0.6559
		16	0.4815

Remarks:

(a) Dependence on λ. It is observed that for large λ, the increase in the error for the same p and N is proportional to $\sqrt{\lambda}$, as predicted by (3.11).

(b) L^2 errors. For some of our calculations, the L^2 errors converged at the rate of $O(h^2)$. In other cases, the convergence rate was lower. We have not yet determined conclusively either by means of computation or analysis what the correct rate should be.

(c) The case p = 0. Although Theorem 3.3 does not predict conver-
gence in this case, computationally, we once again observed O(h) conver-
gence in experiments similar to the above.

(d) Finite Difference Calculations. Computations based on the dif-
ference scheme (4.1) are not reproduced here. They showed similar magni-
tudes of error and identical rates of convergence as the finite element
case, both in the one- and two-dimensional case.

(e) Boundedness of Approximate Solutions. In all our calculations,
we observed that the approximate solution always satisfied $0 \leq u_h \leq 1$.
For the finite difference case, this is justified by Theorem 4.1. For the
finite element case, the discrete maximum principle justifies $u_h \leq 1$, as
shown in Theorem 3.2. We have not, however, been able to prove that
$u_h \geq 0$.

(f) Existence of the Dead Core. In the one-dimensional case, it was
observed computationally that Theorem 2.2 was satisfied with $\lambda_0 = 12$
when p = 0.5. Similar critical values of λ were observed for the two-
dimensional case. In the two-dimensional examples presented, for $\lambda = 4$
there was no dead core, while for other values of λ, a dead core was
observed.

References

[1] Bandle, C., Sperb, R. B. and Stakgold, I., Diffusion and Reaction with Monotone Kinetics, Nonlinear Analysis 8, 321-333 (1984).

[2] Douglas, J., and Dupont, T., A Galerkin method for a nonlinear Dirichlet problem, Math. Comp. 29, 689-696 (1975).

[3] Friedman, A. and Phillips, D., The free boundary of a semilinear elliptic equation, Trans Amer. Math. Soc. 282, 153-182 (1984).

[4] Mittelmann, H. D., On pointwise estimates for a finite element solution of nonlinear boundary value problems, SIAM J. Numer. Anal. 14, 773-778 (1977).

[5] Ortega, I. M. and Rheinboldt, W. C., Iterative solution of non-linear equations in several variables, Academic Press (1970).

[6] Rheinboldt, W.C., On M-functions and their application to nonlinear Gauss-Seidel iterations and to network flows, J. Math Anal. Appl. 32, 274-307 (1970)

[7] Temam, R., Navier-Stokes Equations, Studies in Math and its Applications, Vol. 2, North-Holland (1977).

END

11-87

DTIC